

# Weyl Bogoliubov excitations in Bose-Hubbard extension of Weyl semimetal

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In this paper we study a Bose-Hubbard extension of Weyl semimetal that can be realized for ultracold atoms using laser assisted tunneling and Feshbach resonance technique in three dimensional optical lattices. We present the phase diagram consisting of a superfluid phase and various Mott insulator phases by using Landau theory. The Bogoliubov excitation modes for the weakly interacting case have nontrivial properties (Weyl nodes, bosonic surface arc, et al.) analogs of that in Weyl semimetals of electronic systems, which are smoothly carried over to that of Bloch bands for the noninteracting case. We also explore properties of the insulating phases for the strongly interacting case by calculating both the quasiparticle and quasihole dispersion relation, which shows two quasiparticle spectra touch at Weyl nodes.

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## I. INTRODUCTION AND MOTIVATION

Weyl semimetal (WSM) attracts considerable interest in both theory and experiments recently. Differently from gapped topological insulators and superconductors, WSM has bulk gapless nodal points (dubbed Weyl points), which exhibit topological structure of synthetic monopole in momentum space and give rise to surface Fermi arc that connects different chiral Weyl points. To realize Weyl points, time-reversal and/or inversion symmetry of the system must be broken [1, 2].

Recently, the investigation of topology of bosonic excitation modes attracts increasing attention in interacting bosons in optical lattices [3, 4], magnonic excitations [5–7], phononic excitations [8, 9] and polaritonic excitations [10, 11], etc. The noninteracting bosons condense into the lowest-energy mode at the ground state. However, the energy bands of excited modes exhibit topological structure [3–13], which gives rise to topologically protected edge modes in the excitation spectrum owing to the bulk-boundary relation [4].

Rapid advances on synthetic magnetic and gauge fields in ultracold atoms create opportunities for realizing novel states of matter [14–17]. By using laser-assisted tunneling in three dimensional optical lattices, Tena Dubček et al. proposed that WSM with broken inversion symmetry may be realized in optical lattices [18]. Alongside advances in manipulating ultracold atoms and novel properties of WSM, an interesting issue arises: “what are the properties of excitation modes in superfluid phase and Mott-insulator phases in Bose-Hubbard extension of the Hamiltonian with Weyl points?” Therefore, here we focus on the Bogoliubov excitations of Bose-Hubbard extension of WSM, and find that the energy dispersion relation of excitation modes exhibits Weyl points with chirality and there exist topologically protected bosonic surface-

arc states in both superfluid phase and Mott-insulator phases analogs of that in WSMs of electronic systems.

The remainder of the paper is organized as follows. In Sec. II, we first give the Bose-Hubbard extension of the WSM, and then show the band structure for its noninteracting case. By means of Landau theory, we present phase diagram that consists of superfluid phase and Mott-insulator phases. In Sec. III, we calculate the Bogoliubov excitation bands for bosonic superfluids by using Bogoliubov theory, and present that there are Weyl points analogs of that in WSMs of electronic systems. The bosonic surface-arc states on boundaries are found that connected by Weyl points with different chiralities. In Sec. IV, we derive the quasiparticle and quasihole dispersions in Mott-insulator phase using the functional integral formalism that show two quasiparticle spectra touch at Weyl points. Finally, we conclude our discussions in Sec. V.

## II. BOSE-HUBBARD EXTENSION OF THE WEYL SEMIMETAL

The Hamiltonian of the Bose-Hubbard extension of the WSM in three-dimensional lattices is given by

$$H = H_0 + \frac{U}{2} \sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^{\dagger 2} \hat{a}_{\mathbf{r}}^2 - \mu \sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^{\dagger} \hat{a}_{\mathbf{r}}. \quad (1)$$

Here,  $U$  is the on-site interaction strength,  $\mu$  is the chemical potential, and the Weyl Hamiltonian  $H_0$  takes the following form as [18]

$$H_0 = \sum_{\mathbf{r} \in \mathbf{B}} \left( -J_x \hat{a}_{\mathbf{r}+\delta_x}^{\dagger} \hat{a}_{\mathbf{r}} + J_x \hat{a}_{\mathbf{r}-\delta_x}^{\dagger} \hat{a}_{\mathbf{r}} - J_y \hat{a}_{\mathbf{r}+\delta_y}^{\dagger} \hat{a}_{\mathbf{r}} - J_y \hat{a}_{\mathbf{r}-\delta_y}^{\dagger} \hat{a}_{\mathbf{r}} + h.c. \right) + \sum_{\mathbf{r} \in \mathbf{A}} J_z \hat{a}_{\mathbf{r}+\delta_z}^{\dagger} \hat{a}_{\mathbf{r}} - \sum_{\mathbf{r} \in \mathbf{B}} J_z \hat{a}_{\mathbf{r}+\delta_z}^{\dagger} \hat{a}_{\mathbf{r}} \quad (2)$$

where  $\hat{a}_{\mathbf{r}}$  denotes the bosonic annihilation operator at the lattice site  $\mathbf{r}$  ( $\mathbf{r} \in \mathbf{A}, \mathbf{B}$  sublattices),  $J_x, J_y$  and  $J_z$  are the

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real nearest-neighbor hopping parameters along the  $x$ ,  $y$ , and  $z$  direction, respectively. Here, we introduce vectors  $\delta_{1,2,3}$  given by  $\delta_x = d(1, 0, 0)$ ,  $\delta_y = d(0, 1, 0)$ ,  $\delta_z = d(0, 0, 1)$ , where  $d$  is the length between the neighboring sites. We fix the total number of particles to  $N$ , i.e.,  $\sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}} = N$ .

### A. Bloch band structure for the Weyl semimetal

Firstly, we set  $U = 0$ , and review the band structure of the Hamiltonian with Weyl points in the noninteracting case. Provided that the system has periodic boundary condition, we perform the Fourier transformation

$$\hat{a}_{\mathbf{r}} = \frac{1}{\sqrt{N_{uc}}} \sum_{\mathbf{k}} \hat{a}_{X,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (3)$$

where  $\mathbf{r} \in X = A, B$ , the sum is taken over the discrete momenta  $\mathbf{k}$  in the first Brillouin zone, and  $N_{uc}$  is the number of unit cells in the system. The Hamiltonian (kinetic part) in momentum space is then given by

$$H_{kin} = \sum_{\mathbf{k}} \begin{pmatrix} \hat{a}_{A,\mathbf{k}}^\dagger & \hat{a}_{B,\mathbf{k}}^\dagger \end{pmatrix} \mathcal{H}(\mathbf{k}) \begin{pmatrix} \hat{a}_{A,\mathbf{k}} \\ \hat{a}_{B,\mathbf{k}} \end{pmatrix}. \quad (4)$$

The  $2 \times 2$  hermitian matrix  $\mathcal{H}(\mathbf{k})$  can be described by

$$\mathcal{H}(\mathbf{k}) = \vec{h}(\mathbf{k}) \cdot \vec{\sigma}, \quad (5)$$

where  $I$  is the identity matrix,  $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  are Pauli matrices. The coefficients  $\vec{h}(\mathbf{k}) = (h_1(\mathbf{k}), h_2(\mathbf{k}), h_3(\mathbf{k}))$  are written as

$$\begin{aligned} h_1(\mathbf{k}) &= -2J_y \cos(k_y d), \quad h_2(\mathbf{k}) = -2J_x \sin(k_x d), \\ h_3(\mathbf{k}) &= 2J_z \cos(k_z d). \end{aligned} \quad (6)$$

The two energy bands are obtained through the diagonalization of equation (4) as

$$e_{\pm}(\mathbf{k}) = \pm h(\mathbf{k}) = \pm \sqrt{h_1^2(\mathbf{k}) + h_2^2(\mathbf{k}) + h_3^2(\mathbf{k})}. \quad (7)$$

Hereafter, we choose  $J_x = J_y = J_z = J$ . The system then has four independent Weyl points at  $\{\mathbf{k}_w\} = (0, \pm\pi/2, \pm\pi/2)$ . For non-interacting bosons, BEC into the lowest-energy single-particle states occurs at zero temperature. The bottom of the lowest band  $e_-(\mathbf{k})$  is located at four different momenta of the Brillouin zone  $\{\mathbf{k}_0\} = (\pm\pi/2, 0, 0), (\pm\pi/2, 0, \pi)$ . Here, we consider that the BEC is prepared at  $\mathbf{k}_0 = (\pi/2, 0, 0)$ . At this time, the coefficients  $\vec{h}(\mathbf{k}_0)$  are given by  $(-2J_y, -2J_x, 2J_z)$ .

To determine the single-particle ground state, we parameterize  $\vec{h}(\mathbf{k}_0)$  using the spherical coordinate as

$$\vec{h}(\mathbf{k}_0) = h(\mathbf{k}_0) (\sin \theta_0 \cos \varphi_0, \sin \theta_0 \sin \varphi_0, \cos \theta_0) \quad (8)$$

with  $h(\mathbf{k}_0) = 2\sqrt{3}J$ , and  $(\theta_0, \varphi_0) = (\arccos(1/\sqrt{3}), \arccos[-1/(\sqrt{3}\sin\theta_0)])$ .

### B. Superfluid-Mott insulator transition

After turning on the interaction  $U (> 0)$  between particles, the ground state of the system enters into superfluid (SF) phase with noninteger number of bosons at each site at zero temperature. As interaction increases, qualitatively the interaction between particles will drive the system into Mott insulator (MI) phase if  $U \gg t$ , in which the moving for a particle from one site to another is energetically unfavorable.

In the strong coupling limit, we first introduce a local superfluid order parameter that is written as [19, 20]

$$\psi_{\mathbf{r}} = \langle \hat{a}_{\mathbf{r}}^\dagger \rangle = \langle \hat{a}_{\mathbf{r}} \rangle \quad (9)$$

and with the help of  $\psi_{\mathbf{r}}$ , the hopping term is decoupled into

$$\hat{a}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{j}} = \hat{a}_{\mathbf{r}}^\dagger \psi_{\mathbf{j}} + \psi_{\mathbf{r}} \hat{a}_{\mathbf{j}} - \psi_{\mathbf{r}} \psi_{\mathbf{j}}, \quad (10)$$

where  $\mathbf{j}$  denotes the coordinate of lattice site  $\mathbf{r}$ 's nearest neighbor site. Then the Hamiltonian takes following form:

$$\begin{aligned} \hat{H}^{eff} &= \sum_{\mathbf{r} \in \mathbf{B}} -J_x (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_x} \\ &\quad - J_y (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_y} - J_z (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_z} \\ &\quad + \sum_{\mathbf{r} \in \mathbf{A}} J_x (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_x} \\ &\quad - J_y (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_y} + J_z (\hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger - \psi_{\mathbf{r}}) \psi_{\mathbf{r}+\delta_z} \\ &\quad + \frac{U}{2} \sum_{\mathbf{r}} n_{\mathbf{r}} (n_{\mathbf{r}} - 1) - \mu \sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}}. \end{aligned} \quad (11)$$

In the system, owing to that there are two kinds of lattices, i.e.,  $\mathbf{A}$ -sublattice and  $\mathbf{B}$ -sublattice, we define order parameters as  $\psi_{\mathbf{r} \in \mathbf{A}} \equiv \psi_1$  and  $\psi_{\mathbf{r} \in \mathbf{B}} \equiv \psi_2$ , respectively. Then the effective onsite Hamiltonian  $\hat{H}_{on}^{eff}$  is given by

$$\begin{aligned} \hat{H}_{on}^{eff} &= J_x (\hat{a}_1^\dagger + \hat{a}_1) \psi_2 - J_x (\hat{a}_2^\dagger + \hat{a}_2) \psi_1 \\ &\quad - J_y (\hat{a}_1^\dagger + \hat{a}_1) \psi_2 - J_y (\hat{a}_2^\dagger + \hat{a}_2) \psi_1 + 2J_y \psi_1 \psi_2 \\ &\quad + J_z (\hat{a}_1^\dagger + \hat{a}_1) \psi_1 - J_z (\hat{a}_2^\dagger + \hat{a}_2) \psi_2 \\ &\quad + J_z (\psi_2^2 - \psi_1^2) + \frac{\bar{U}}{2} (n_1^2 + n_2^2 - n) - \bar{\mu} n \end{aligned} \quad (12)$$

where  $a_{\mathbf{r} \in \mathbf{A}} = a_1$ ,  $a_{\mathbf{r} \in \mathbf{B}} = a_2$ ,  $\bar{U} = U/z$ , and  $\bar{\mu} = \mu/z$ , and  $z = 2$  is the number of nearest-neighbor sites in one direction. Next, we write  $\hat{H}_{on} = \hat{H}_{on}^0 + \hat{H}_{on}'$  with

$$\begin{aligned} \hat{H}_{on}^0 &= \frac{\bar{U}}{2} \sum (n_1^2 + n_2^2 - n) - \bar{\mu} n \\ &\quad + 2J_y \psi_1 \psi_2 + J_z (\psi_2^2 - \psi_1^2) \end{aligned} \quad (13)$$

and

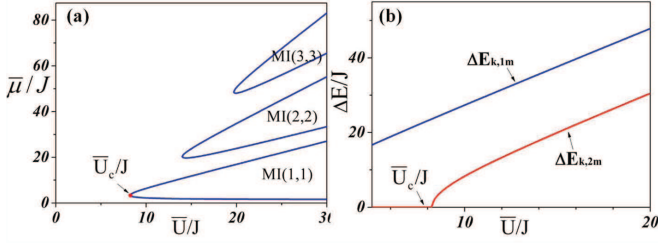


FIG. 1: (Color online) (a) Phase diagram of the Bose-Hubbard extension of WSM. The vertical axis and horizontal axis show the dimensionless chemical potential  $\bar{\mu} = \mu/z$  and  $\bar{U} = U/z$ , respectively. (b) The first-order approximations to the dispersion of the density fluctuations.

$$\begin{aligned} \hat{H}'_{on} = & J_x(\hat{a}_1^\dagger + \hat{a}_1)\psi_2 - J_x(\hat{a}_2^\dagger + \hat{a}_2)\psi_1 \\ & - J_y(\hat{a}_1^\dagger + \hat{a}_1)\psi_2 - J_y(\hat{a}_2^\dagger + \hat{a}_2)\psi_1 \\ & + J_z(\hat{a}_1^\dagger + \hat{a}_1)\psi_1 - J_z(\hat{a}_2^\dagger + \hat{a}_2)\psi_2. \end{aligned} \quad (14)$$

In the occupation numbers basis, we can find that the odd powers of the expansion of energy is always zero. Hence, the energy for the zero-order terms is then given by

$$\begin{aligned} E_g^{(0)} = & \min(e_{\{n_1, n_2\}}^{(0)}) \\ = & \frac{\bar{U}}{2}(n_1^2 + n_2^2 - n) - \bar{\mu}n \\ & + 2J_y\psi_1\psi_2 + J_z(\psi_2^2 - \psi_1^2), \end{aligned} \quad (15)$$

and the energy for the second-order perturbation is

$$E_n^{(2)} = \frac{\langle n_1; n_2 | H' | k_1; k_2 \rangle \langle k_1; k_2 | H' | n_1; n_2 \rangle}{E_n^{(0)} - E_k^{(0)}}, \quad (16)$$

where  $k_1 = n_1 + 1$ ,  $k_2 = n_2$  or  $k_1 = n_1$ ,  $k_2 = n_2 + 1$ . After direct calculations, we obtain

$$\begin{aligned} E_n^{(2)} = & \frac{n_1(J_x\psi_2 - J_y\psi_2 + J_z\psi_1)^2}{(n_1 - 1)\bar{U} - \bar{\mu}} \\ & + \frac{(n_1 + 1)(J_x\psi_2 - J_y\psi_2 + J_z\psi_1)^2}{-n_1\bar{U} + \bar{\mu}} \\ & + \frac{n_2(-J_x\psi_1 - J_y\psi_1 - J_z\psi_2)^2}{(n_2 - 1)\bar{U} - \bar{\mu}} \\ & + \frac{(n_2 + 1)(-J_x\psi_1 - J_y\psi_1 - J_z\psi_2)^2}{-n_2\bar{U} + \bar{\mu}} \end{aligned} \quad (17)$$

In summary, the ground-state energy for the system in terms of  $\psi$  is given by

$$\begin{aligned} E_g \simeq & E_g^{(0)} + E_n^{(2)} \\ = & a_0 + a_2\psi_1^2 + c_2\psi_1\psi_2 + b_2\psi_2^2 + \dots \end{aligned} \quad (18)$$

where

$$\begin{aligned} a_0 = & \frac{\bar{U}}{2}(n_1^2 + n_2^2 - n) - \bar{\mu}n, \\ a_2 = & -J_z + \frac{(-\bar{U} - \mu)J_z^2}{[(n_1 - 1)\bar{U} - \bar{\mu}][ -n_1\bar{U} + \bar{\mu}]} \\ & + \frac{(-\bar{U} - \bar{\mu})(J_x + J_y)^2}{[(n_2 - 1)\bar{U} - \bar{\mu}][ -n_2\bar{U} + \bar{\mu}]}, \\ b_2 = & J_z + \frac{(-\bar{U} - \bar{\mu})(J_x - J_y)^2}{[(n_1 - 1)\bar{U} - \bar{\mu}][ -n_1\bar{U} + \bar{\mu}]} \\ & + \frac{(-\bar{U} - \bar{\mu})J_z^2}{[(n_2 - 1)\bar{U} - \bar{\mu}][ -n_2\bar{U} + \bar{\mu}]}, \\ c_2 = & 2J_y + \frac{2(-\bar{U} - \bar{\mu})(J_x - J_y)J_z}{[(n_1 - 1)\bar{U} - \bar{\mu}][ -n_1\bar{U} + \bar{\mu}]} \\ & + \frac{2(-\bar{U} - \bar{\mu})(J_x + J_y)J_z}{[(n_2 - 1)\bar{U} - \bar{\mu}][ -n_2\bar{U} + \bar{\mu}]}. \end{aligned}$$

Differently from conventional Landau theory of phase transitions, in this case, the system have two order parameters. Based on the geometry knowledge, when the Gaussian curvature of the energy-order parameters surface is zero at the point  $\psi_1 = \psi_2 = 0$ , the phase transition occurs. Therefore, we can obtain a function of phase-transition line readily by

$$\frac{\partial^2 E}{\partial \tilde{\psi}_1^2} \Big|_{(0,0)} \frac{\partial^2 E}{\partial \tilde{\psi}_2^2} \Big|_{(0,0)} - \left( \frac{\partial^2 E}{\partial \tilde{\psi}_1 \partial \tilde{\psi}_2} \Big|_{(0,0)} \right)^2 = 0, \quad (19)$$

which leads to

$$4a_2b_2 - c_2^2 = 0 \quad (20)$$

Solving the equation (20), yields

$$\begin{aligned} \bar{\mu} = & \frac{1}{2} \left[ -\sqrt{2} + (2n - 1)\bar{U} \right. \\ & \left. \pm \sqrt{2 - 2\sqrt{2}\bar{U} - 4\sqrt{2}n\bar{U} + \bar{U}^2} \right] \end{aligned} \quad (21)$$

with  $n \equiv n_1 = n_2$ . Correspondingly, the point of smallest  $\bar{U}$  (denoted by  $\bar{U}_c$ ) for each lobe is

$$\bar{U}_c = \sqrt{2} + 2\sqrt{2}n + 2\sqrt{2n + 2n^2}. \quad (22)$$

In conclusion, by applying the Landau theory of phase transitions that treats the interactions exactly and the hopping terms as perturbation, we get the SF-MI phase transition diagram in Fig. 1 (a). It shows that the phase transition point  $\bar{U}_c/J \approx 8.25$  for the MI (1, 1) lobe.

For smaller  $U < U_c$ , the system is in the SF phase. According to the Hugenholtz-Pines theorem, there are always gapless density fluctuations. In the followings, we will study the excitation modes in SF phase.

### III. BOGOLIUBOV THEORY AND TOPOLOGY OF EXCITATION MODES FOR SUPERFLUID

#### A. Bogoliubov theory

In this section, we present the Bogoliubov theory for homogeneous condensates with weak repulsive interactions  $U > 0$ , and determine the band structure of Bogoliubov excitations. Here, “homogeneous” case refers to the situation where the system has the periodicity of the lattice. We then study the topology of Bogoliubov excitations, and determine whether the excitations have novel properties.

By means of the Gross-Pitaevskii (GP) theory, we derive a condensate wave function to formulate the Bogoliubov theory for the boson system. In the GP theory, we first introduce the GP energy function  $E$  by replacing  $(\hat{a}(\mathbf{r}), \hat{a}^\dagger(\mathbf{r}))$  by  $(\psi(r), \psi^\dagger(r))$  in the Hamiltonian (2), and minimize it with respect to  $(\psi(r), \psi^\dagger(r))$  under the constraint  $\sum_r |\psi(r)|^2 = N$ . Since the single-particle ground state is formed at  $k = 0$ , we introduce the following homogeneous ansatz for the interacting case:

$$\psi(r) = \frac{1}{\sqrt{N_{uc}}} \psi_x. \quad (23)$$

Next, we introduced the chemical potential  $\mu$  as a Lagrange multiplier to satisfy the particle-number constraint. The functional to be minimized is then given by

$$E - \mu N = (\psi_A^*, \psi_B^*) [\mathcal{H}(\mathbf{k}_0) - \mu I] \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + \frac{U}{N_{uc}} (|\psi_A|^4 + |\psi_B|^4). \quad (24)$$

Minimizing this with respect to  $\psi_x^*$  ( $x \in A, B$ ) gives a homogeneous version of the GP equations:

$$[\mathcal{H}(\mathbf{k}_0) - \mu I] \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + \frac{U}{N_{uc}} \begin{pmatrix} \psi_A^* \psi_A^2 \\ \psi_B^* \psi_B^2 \end{pmatrix} = 0. \quad (25)$$

Since the single-particle ground state is created by  $a_-^\dagger(\mathbf{k}_0)$ , it is convenient to parameterize  $(\psi_A, \psi_B)^T$  as

$$\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \sqrt{N} \begin{pmatrix} f_A \\ f_B \end{pmatrix} = \sqrt{N} \begin{pmatrix} -e^{-i\varphi} \sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2}) \end{pmatrix}, \quad (26)$$

where  $\theta = \theta_0$  when  $U = 0$ . Multiplying equation (25) by  $(f_A^*, f_B^*)$  or  $(-f_B^*, f_A^*)$  from the left, we get

$$-h(\mathbf{k}_0) [\cos \theta_0 \cos \theta + \sin \theta_0 \sin \theta \cos(\varphi_0 - \varphi)] + 2Un (|f_A|^4 + |f_B|^4) = \mu, \quad (27)$$

$$h(\mathbf{k}_0) (\cos \theta_0 \sin \theta \cos \varphi - \sin \theta_0 \cos \varphi_0 \cos \theta) - Un \cos \varphi \sin \theta \cos \theta = 0, \quad (28)$$

$$h(\mathbf{k}_0) \sin \theta_0 \sin \varphi_0 + \mu \sin \theta \sin \varphi - Un \sin \theta \sin \varphi = 0 \quad (29)$$

where  $n := N/(2N_{uc})$ .

We now discuss excitations from the condensate ground state by using the Bogoliubov theory. Using equation (3), we decompose  $\hat{\mathbf{a}}_{\mathbf{r}}$  into the condensate and noncondensate parts as

$$\begin{aligned} \hat{\mathbf{a}}_{\mathbf{r}} &= \frac{1}{\sqrt{N_{uc}}} \hat{\mathbf{a}}_{X,0} + \frac{1}{\sqrt{N_{uc}}} \sum_{\mathbf{k} \neq 0} \hat{\mathbf{a}}_{X,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \\ &= \frac{1}{\sqrt{N_{uc}}} (f_X \hat{\mathbf{a}}_- - \epsilon_X f_{\bar{X}} \hat{\mathbf{a}}_+) + \frac{1}{\sqrt{N_{uc}}} \sum_{\mathbf{k} \neq 0} \hat{\mathbf{a}}_{X,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \\ &= \frac{1}{\sqrt{N_{uc}}} f_X \hat{\mathbf{a}}_- + \tilde{\mathbf{a}}(\mathbf{r}), \end{aligned} \quad (30)$$

where  $\tilde{\mathbf{a}}(\mathbf{r}) = \frac{1}{\sqrt{N_{uc}}} [-\epsilon_X f_{\bar{X}} \hat{\mathbf{a}}_+ + \sum_{\mathbf{k} \neq 0} \hat{\mathbf{a}}_{X,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}}]$  with  $\bar{A} = B$  and  $\bar{B} = A$ . Following the Bogoliubov approximation, we replace both  $\hat{\mathbf{a}}_-$  and  $\hat{\mathbf{a}}_+^\dagger$  by  $\sqrt{N}$ , and substitute equation (30) into  $H - \mu N$  up to quadratic order in  $\tilde{\mathbf{a}}(\mathbf{r})$ . The terms linear in  $\tilde{\mathbf{a}}(\mathbf{r})$  or  $\tilde{\mathbf{a}}^\dagger(\mathbf{r})$  disappear because of the stability condition of the condensate in equation (28),

and we arrive at the Bogoliubov Hamiltonian

$$H - \mu N = \frac{1}{2} (\hat{\mathbf{a}}_+^\dagger, \hat{\mathbf{a}}_+) M_+ \begin{pmatrix} \hat{\mathbf{a}}_+ \\ \hat{\mathbf{a}}_+^\dagger \end{pmatrix} + \frac{1}{2} \sum_{\mathbf{k} \neq 0} \hat{\alpha}_k^\dagger M(k) \hat{\alpha}_k \quad (31)$$

with  $\hat{\alpha}_k^\dagger = (\hat{\mathbf{a}}_{A,\mathbf{k}}^\dagger, \hat{\mathbf{a}}_{B,\mathbf{k}}^\dagger, \hat{\mathbf{a}}_{A,-\mathbf{k}}, \hat{\mathbf{a}}_{B,-\mathbf{k}})$ . Here, the  $2 \times 2$  matrix  $M_+$  and  $4 \times 4$  matrix  $M(k)$  are given by

$$M_+ = [h(0) \cos(\theta - \theta_0) - \mu + 8Un f_A^2 f_B^2] I + 4Un f_A^2 f_B^2 \sigma_1,$$

and

$$M(k) = \begin{pmatrix} \mathcal{H}(\mathbf{k}) - \mu I + 4Un |F|^2 & 2Un F^2 \\ 2Un F^{*2} & \mathcal{H}^T(-\mathbf{k}) - \mu I + 4Un |F|^2 \end{pmatrix}.$$

Here,  $F := \text{diag}(f_A, f_B)$ .

To diagonalize above Bogoliubov Hamiltonian, we perform generalized Bogoliubov transformations as

$$\begin{pmatrix} \hat{\mathbf{a}}_+ \\ \hat{\mathbf{a}}_+^\dagger \end{pmatrix} = W_+ \begin{pmatrix} \hat{\mathbf{b}}_+(0) \\ \hat{\mathbf{b}}_+^\dagger(0) \end{pmatrix}, \quad \hat{\alpha}_k = W(k) \hat{\beta}_k \quad (32)$$

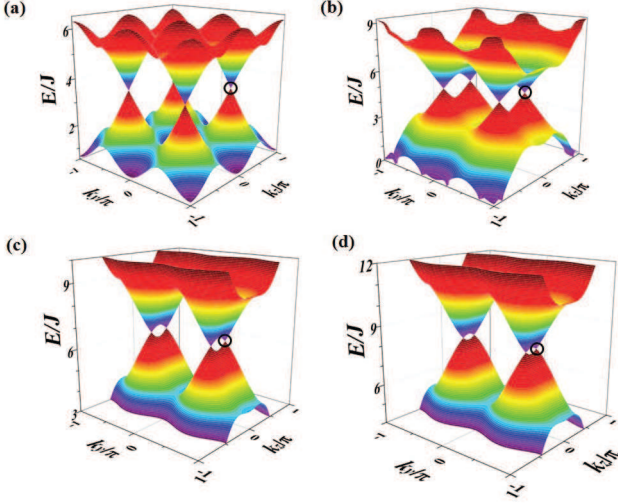


FIG. 2: (Color online) The energy spectra of Bogoliubov quasiparticles with fixed  $k_x = 0$  and (a)  $\bar{U}n/J = 0.0$ ; (b)  $\bar{U}n/J = 1.0$ ; (c)  $\bar{U}n/J = 3.0$ ; (d)  $\bar{U}n/J = 5.0$ .

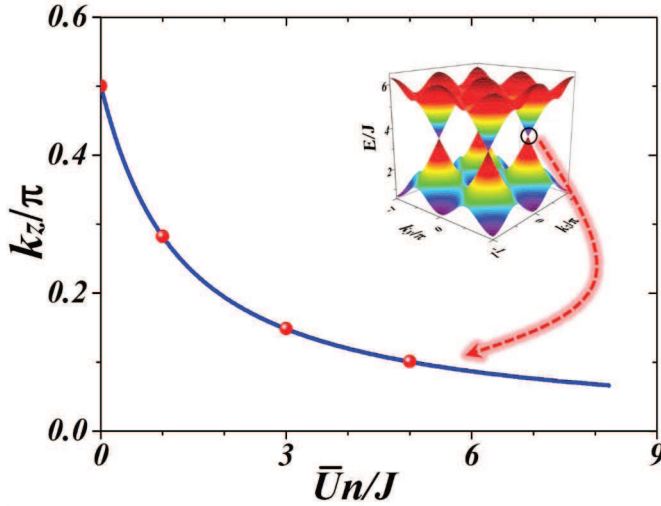


FIG. 3: (Color online) The location of the Weyl point indicated by the black circle in the inset versus  $\bar{U}n$ . The  $k_z$ -coordinates of Weyl points in figure 2 are indicated by red points. In particular, when  $U = 0$ , the considered Weyl point locates at the momentum point  $(0, \pi/2, \pi/2)$

with

$$\hat{\beta}_k^\dagger = (\hat{b}_{+,k}^\dagger, \hat{b}_{-,k}^\dagger, \hat{b}_{+,-k}, \hat{b}_{-,-k}).$$

Here,  $W_+$  and  $W(k)$  are paraunitary matrices which satisfy

$$\begin{aligned} W_+^\dagger \sigma_3 W_+ &= W_+ \sigma_3 W_+^\dagger = \sigma_3, \\ W_k^\dagger \tau_3 W_k &= W_k \tau_3 W_k^\dagger = \tau_3 \end{aligned} \quad (33)$$

with  $\tau_3 = \text{diag}(1, 1, -1, -1)$ . These equations ensure the invariance of the bosonic commutation relations for

Bogoliubov excitations. If the matrices  $W_+$  and  $W_k$  are chosen to satisfy

$$W_+^\dagger M_+ W_+ = E_+(0) I,$$

and

$$W_k^\dagger M(k) W_k = \text{diag}(E_{+,k}, E_{-,k}, E_{+,-k}, E_{-,-k}),$$

the Bogoliubov Hamiltonian is diagonalized as

$$H - \mu N = \sum_{\mathbf{k}} E_{+,k} \hat{b}_{+,k}^\dagger \hat{b}_{+,k} + \sum_{\mathbf{k} \neq 0} E_{-,k} \hat{b}_{-,k}^\dagger \hat{b}_{-,k} + \text{const.} \quad (34)$$

The  $4 \times 4$  paraunitary matrix  $W_k$  can be constructed numerically, which is written in the form

$$W_k = \begin{pmatrix} U(k) & V^*(-k) \\ V(k) & U^*(-k) \end{pmatrix}, \quad (35)$$

where

$$U(k) = \begin{pmatrix} \alpha_{A,+}(k) & \alpha_{A,-}(k) \\ \alpha_{B,+}(k) & \alpha_{B,-}(k) \end{pmatrix},$$

and

$$V(k) = \begin{pmatrix} \beta_{A,+}(k) & \beta_{A,-}(k) \\ \beta_{B,+}(k) & \beta_{B,-}(k) \end{pmatrix}.$$

Provided that a Hermite matrix  $H(\mathbf{k})$  is unitarily equivalent to a positive-definite diagonal matrix, a paraunitary matrix  $W_k$  can be obtained by a method based on the Cholesky decomposition [5, 6, 21]. In this method, we first decompose  $H(\mathbf{k})$  into a product between upper triangle matrix  $K_k$  and its Hermite conjugate  $K_k^\dagger$ , i.e.,  $H(\mathbf{k}) = K_k^\dagger K_k$ . The unitarily positive definiteness of  $H(\mathbf{k})$  always allows this decomposition and also guarantees the existence of  $K_k^{-1}$ . We next introduce a unitary matrix  $U_k$  which diagonalizes a Hermite matrix  $T_k \equiv K_k \sigma_3 K_k^\dagger$ , and then

$$U_k^\dagger T_k U_k = \begin{pmatrix} E_k & \\ & -E_{-k} \end{pmatrix}. \quad (36)$$

By direct numerical calculations, we get the Bogoliubov excitation bands  $E_\pm(k)$  as shown in Fig. 2. It shows that there are Weyl points in the excitation band. As the interaction strength increases, Weyl points approach gradually with each other along the  $k_z$ -direction (see Fig. 3)

## B. Berry Curvature

To study the topological properties of excitation modes of Bogoliubov quasiparticles, we define the basis vectors of  $M(k)$  as

$$|w_\lambda(k)\rangle = (\alpha_{A,\lambda}(k), \alpha_{B,\lambda}(k), \beta_{A,\lambda}(k), \beta_{B,\lambda}(k))^T$$



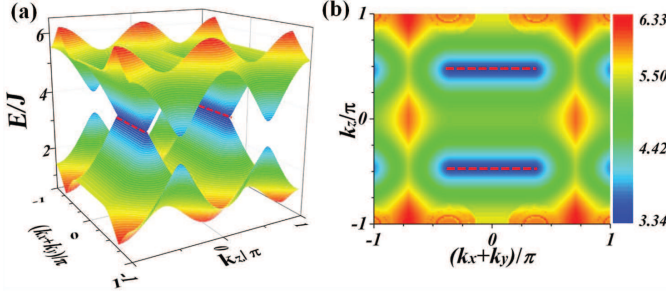


FIG. 4: (Color online) (a) The Bogoliubov spectra of slab with finite width. The bosonic surface-arc states are indicated by red dashed lines. (b) The contour plot of upper energy spectra of excitation modes for BECs in a slab with finite width along planes orthogonal to the  $\vec{x} - \vec{y}$  direction. The arc states are indicated by red dashed lines. In both (a) and (b), the parameter  $\bar{U}n/J = 0.2$ .

with  $\lambda = \pm$ , of which  $\langle w_{\lambda'}(k) | \tau_3 | w_{\lambda}(k) \rangle = \delta_{\lambda'\lambda}$ . We then have  $M(k) | w_{\lambda}(k) \rangle = E_{\lambda}(k) \tau_3 | w_{\lambda}(k) \rangle$ , and the Berry curvature takes the form

$$B_{\lambda,k}(\mathbf{k}) = i\epsilon_{ijk} \langle \partial_i w_{\lambda}(\mathbf{k}) | \tau_3 | \partial_j w_{\lambda}(\mathbf{k}) \rangle \quad (37)$$

with  $\partial_j = \partial/\partial k_j$  and  $j = x, y, z$ . It shows a synthetic magnetic monopole located at  $\{\mathbf{k}_w\}$ . The topology of Weyl point is characterized by the first Chern number defined by  $C_{\mathbf{k}_w,-} = \oint d\mathbf{S} \cdot \mathbf{B}_-(\mathbf{k})$ , which is calculated by the integral of Berry curvature throughout the surface enclosing the Weyl point. After direct calculations, we obtain  $C_{\mathbf{k}_w,-} = \pm 1$  which implies that Weyl points have different chiralities.

### C. Bosonic Surface States

We apply the BdG theory to study the Bogoliubov excitations of superfluids by choosing a slab with finite width along planes orthogonal to the  $\vec{x} - \vec{y}$  direction, which has sharp the boundaries. The energy spectra and contour plot of upper energy spectra of excitation modes are shown in Fig. 4(a) and (b), respectively. We see there are topologically protected surface states (dubbed bosonic arcs) of excitation modes which are the analogs of Fermi arcs in electronic systems. As the interaction increases, two arcs connected by two Weyl points will approach gradually with each other along the  $k_z$ -direction.

## IV. EXCITATIONS IN MOTT INSULATOR PHASE

In this section, we apply a path integral formulation to calculate the excitation spectra of the MI state in the strong coupling regime [20]. We first write the partition function for the Bose-Hubbard extension in terms of path integral as  $Z = \int \mathcal{D}a^* \mathcal{D}a \exp \{-S[a^*, a]/\hbar\}$ , where the action is given by

$$S[a^*, a] = \int_0^\beta d\tau \left[ \sum_{\mathbf{r}} a_{\mathbf{r}}^*(\tau) (\hbar \partial_\tau - \mu) a_{\mathbf{r}}(\tau) + H_0(\tau) \right] + \frac{1}{2} U \sum_{\mathbf{r}} a_{\mathbf{r}}^*(\tau) a_{\mathbf{r}}^*(\tau) a_{\mathbf{r}}(\tau) a_{\mathbf{r}}(\tau) \quad (38)$$

with  $\beta = \frac{1}{k_B T}$ ,  $k_B$  is the Boltzman constant, and  $H_0(\tau)$  is obtained by replacing the bosonic operators ( $\hat{a}_{\mathbf{r}}^\dagger, \hat{a}_{\mathbf{r}}$ ) in Eq. (2) by complex functions ( $a_{\mathbf{r}}^*(\tau), a_{\mathbf{r}}(\tau)$ ). For convenience, in following we denote  $H_0(\tau)$  (hopping terms) as  $\sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} a_{\mathbf{r}}^* a_{\mathbf{j}}$  that are perturbation terms in strong coupling regime, where  $J_{\mathbf{rj}}$  denotes real nearest-neighbor hopping parameters along the  $x, y$ , and  $z$  direction. In order to decouple the hopping terms, we make use of Hubbard-Stratonovich transformation and rewrite the action as

$$S[a^*, a, \psi^*, \psi] = S[a^*, a] + \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} (\psi_{\mathbf{r}}^* - a_{\mathbf{r}}^*) J_{\mathbf{rj}} (\psi_{\mathbf{j}} - a_{\mathbf{j}}), \quad (39)$$

where  $\psi^*$  and  $\psi$  are the order parameter fields. After direct calculations, the effective action then becomes

$$S[a^*, a, \psi^*, \psi] = \int_0^{\hbar\beta} d\tau \left[ \sum_{\mathbf{r}} a_{\mathbf{r}}^* (\hbar \frac{\partial}{\partial \tau} - \mu) a_{\mathbf{r}} + \frac{1}{2} U \sum_{\mathbf{r}} a_{\mathbf{r}}^{*2} \times a_{\mathbf{r}}^2 - \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} (a_{\mathbf{r}}^* \psi_{\mathbf{j}} + \psi_{\mathbf{r}}^* a_{\mathbf{j}}) + \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} \psi_{\mathbf{r}}^* \psi_{\mathbf{j}} \right]. \quad (40)$$

By performing integration over the complex fields  $a_{\mathbf{r}}^*$  and  $a_{\mathbf{r}}$ , Then, we have the explicit form

$$e^{-S^{eff}[\psi^*, \psi]} = \exp \left( -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} \psi_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau) \right) \\ \times \int \mathcal{D}a^* \mathcal{D}a \exp \left\{ -S^{(0)}[a^*, a] / \hbar - \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \right\} \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left( -\sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} (a_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau) + \psi_{\mathbf{r}}^*(\tau) a_{\mathbf{j}}(\tau)) \right) \right\}, \quad (41)$$


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where we have denoted the action for  $J_{\mathbf{rj}} = 0$  by  $S^{(0)}[a^*, a]$ .

Now by using the relation  $\langle e^{A_i} \rangle = e^{\langle A_i \rangle + \frac{1}{2}(\langle A_i^2 \rangle - \langle A_i \rangle^2) + \dots}$ , we can get the expressions for the action  $S^{eff}[\psi^*, \psi]$  up to the second order, i.e.,

$$S^{eff}[\psi^*, \psi] \approx S^{(0)}[\psi^*, \psi] + S^{(2)}[\psi^*, \psi],$$

where  $S^{(2)}[\psi^*, \psi]$  is given by

$$S^{(2)}[\psi^*, \psi] = \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} \psi_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau) - \frac{1}{2\hbar} \left\langle \left( \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} [a_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau) + \psi_{\mathbf{r}}^*(\tau) a_{\mathbf{j}}(\tau)] \right)^2 \right\rangle_{S^{(0)}} \\ = -\frac{1}{2\hbar} \left\langle \int_0^{\hbar\beta} \int_0^{\hbar\beta} d\tau d\tau' \sum_{\mathbf{r}, \mathbf{j}, \mathbf{r}', \mathbf{j}'} J_{\mathbf{rj}} J_{\mathbf{r}'\mathbf{j}'} [a_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau) + \psi_{\mathbf{r}}^*(\tau) a_{\mathbf{j}}(\tau)] [a_{\mathbf{r}'}^*(\tau') \psi_{\mathbf{j}'}(\tau') + \psi_{\mathbf{r}'}^*(\tau') a_{\mathbf{j}'}(\tau')] \right\rangle_{S^{(0)}} \\ + \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} J_{\mathbf{rj}} \psi_{\mathbf{r}}^*(\tau) \psi_{\mathbf{j}}(\tau). \quad (42)$$


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According to the correlations, i.e.,

we have the action  $S^{(2)}[\psi^*, \psi]$ , i.e.,

$$\langle a_{\mathbf{r}}^* a_{\mathbf{j}} \rangle_{S^{(0)}} = \langle a_{\mathbf{r}} a_{\mathbf{j}} \rangle_{S^{(0)}} = 0, \\ \langle a_{\mathbf{r}}^* a_{\mathbf{j}} \rangle_{S^{(0)}} = \langle a_{\mathbf{r}} a_{\mathbf{j}}^* \rangle_{S^{(0)}} = \langle a_{\mathbf{r}} a_{\mathbf{j}}^* \rangle_{S^{(0)}} \delta_{\mathbf{rj}},$$


---

$$S^{(2)}[\psi^*, \psi] = \int_0^{\hbar\beta} d\tau \sum_{\mathbf{r}, \mathbf{j}} \psi_{\mathbf{r}}^* J_{\mathbf{rj}} \psi_{\mathbf{j}} - \frac{1}{\hbar} \int_0^{\hbar\beta} \int_0^{\hbar\beta} d\tau d\tau' \sum_{\mathbf{r}, \mathbf{j}, \mathbf{r}', \mathbf{j}'} J_{\mathbf{rj}} J_{\mathbf{r}'\mathbf{j}'} \psi_{\mathbf{j}}^*(\tau) \left\langle T_{\tau} [a_{\mathbf{r}}(\tau) a_{\mathbf{r}'}^*(\tau')] \right\rangle_{S^{(0)}} \psi_{\mathbf{j}'}(\tau'). \quad (43)$$


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For the quadratic term, we can get the formulation in momentum space by using Fourier transformation, i.e.,

with  $A = -B = 2J_z \cos(k_z)$  and  $C = -2J_y \cos(k_y) + i2J_x \cos(k_x)$ . Near the phase transformation point,  $S^{(0)}$  is going zero. Therefore, the effective action becomes

$$\sum_{ijj'} t_{ij} t_{ij'} \psi_j^*(\tau) \psi_{j'}(\tau') = \sum_k \Psi_k^*(\tau) \mathcal{H}^2 \Psi_k^*(\tau'), \quad (44)$$

where  $\Psi_k^*(\tau) = (\psi_{Ak}^*(\tau), \psi_{Bk}^*(\tau))$  and

$$\mathcal{H} = \begin{pmatrix} A & C^* \\ C & B \end{pmatrix} \quad (45)$$

$$S^{eff} = \int_0^{\hbar\beta} \sum_k \Psi_k^*(\tau) \mathcal{H} \Psi_k(\tau') - \frac{1}{\hbar} \int_0^{\hbar\beta} \int_0^{\hbar\beta} d\tau d\tau' \left\langle a_{\mathbf{r}}(\tau) a_{\mathbf{r}'}^*(\tau') \right\rangle \sum_k \Psi_k^*(\tau) \mathcal{H}^2 \Psi_k(\tau') \quad (46)$$

with  $\left\langle a_{\mathbf{r}}(\tau) a_{\mathbf{r}'}^*(\tau') \right\rangle_{S^{(0)}} = \left\langle T_{\tau} \left[ a_{\mathbf{r}}(\tau) a_{\mathbf{r}'}^*(\tau') \right] \right\rangle_{S^{(0)}}$ . Because the time ordering can be expressed by Matsubara Green function

$$\begin{aligned} \left\langle T_{\tau} \left[ a_i(\tau) a_{i'}^*(\tau') \right] \right\rangle_{S^{(0)}} &= \theta(\tau - \tau') \left\langle a_i(\tau) a_{i'}^{\dagger}(\tau') \right\rangle_{S^{(0)}} \\ &+ \theta(\tau - \tau') \left\langle a_{i'}^{\dagger}(\tau') a_i(\tau) \right\rangle_{S^{(0)}}, \end{aligned} \quad (47)$$

we find

$$\begin{aligned} \left\langle a_i(\tau) a_{i'}^*(\tau') \right\rangle_{S^{(0)}} &= \theta(\tau - \tau') (n+1) e^{-(\mu+nU)(\tau-\tau')/\hbar} \\ &+ \theta(\tau - \tau') n e^{(\mu-(n-1)U)(\tau'-\tau)/\hbar} \end{aligned} \quad (48)$$

By introducing Matsubara frequencies, the  $\psi_{Ak}$  and  $\psi_{Bk}$  then becomes

$$\begin{aligned} \psi_{Ak}(\tau) &= \frac{1}{\sqrt{\hbar\beta}} \sum_m e^{-i\omega\tau} \psi_{Ak,\omega_m}, \\ \psi_{Bk}(\tau) &= \frac{1}{\sqrt{\hbar\beta}} \sum_m e^{-i\omega\tau} \psi_{Bk,\omega_m}. \end{aligned} \quad (49)$$

At last, we can readily get the action near the phase transition point as

$$\begin{aligned} S^{eff}[\psi^*, \psi] &= \sum_{k,m} \Psi_k^* (\mathcal{H} - \mathcal{H}^2 f_{\omega_m}) \Psi_k \\ &= \sum_{k,m} \Psi_k^* [-\hbar G^{-1}(k, i\omega_m)] \Psi_k, \end{aligned} \quad (50)$$

where  $\Psi_k^* = (\psi_{Ak,\omega_m}^*, \psi_{Bk,\omega_m}^*)$ , and

$$f_{\omega_m} = \frac{n+1}{-i\hbar\omega_m - \mu + nU} + \frac{n}{i\hbar\omega_m + \mu - (n-1)U}. \quad (51)$$

Under the usual analytic continuation  $i\omega_m \rightarrow \omega_m$ , we can obtain a function of real energies  $\hbar\omega$ , i.e.,

$$\det[G^{-1}] = 0. \quad (52)$$

Then quasiparticle and quasihole dispersion relations are given by

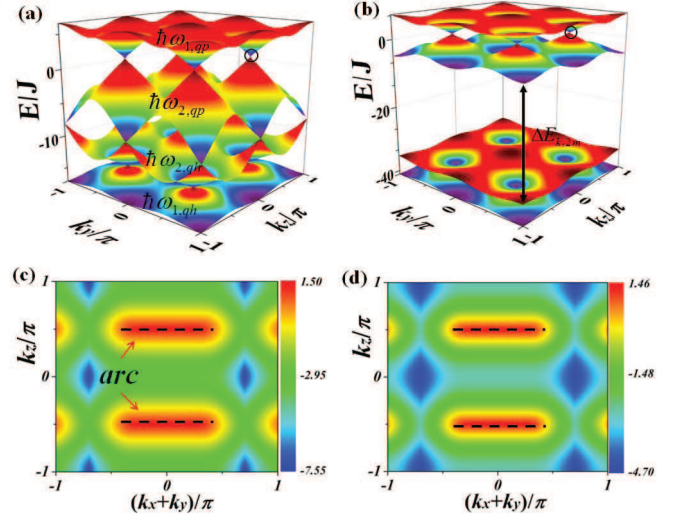


FIG. 5: (Color online) The energy spectra of quasiparticle and quasihole excitations with fixed  $k_x = 0$  for (a)  $\bar{U}/J = 8.25$  and (b)  $\bar{U}/J = 20.0$  in MI(1,1) phase; and the contour plot of energy spectra of lower one of quasiparticle-excitation modes in MI(1,1) phase in a slab with finite width along planes orthogonal to the  $\vec{x} - \vec{y}$  direction for (c)  $\bar{U}/J = 8.25$  and (d)  $\bar{U}/J = 20.0$  in MI(1,1) phase. The locations of the Weyl nodes are shown indicated by black circles in (a) and (b). The bosonic arc states are indicated by black dashed lines in (c) and (d).

$$\begin{aligned} \hbar\omega_{1,qp,ph} &= \frac{1}{2} \left[ -2\mu + (2n-1)U - \frac{1}{f_{\omega_{m+}}} \pm \Delta E_{k1} \right], \\ \hbar\omega_{2,qp,ph} &= \frac{1}{2} \left[ -2\mu + (2n-1)U - \frac{1}{f_{\omega_{m-}}} \pm \Delta E_{k2} \right], \end{aligned} \quad (53)$$

where

$$\begin{aligned} \Delta E_{k,1} &= \sqrt{U^2 - \frac{(4n+2)U}{f_{\omega_{m+}}} + \frac{1}{f_{\omega_{m+}}^2}}, \\ \Delta E_{k,2} &= \sqrt{U^2 - \frac{(4n+2)U}{f_{\omega_{m-}}} + \frac{1}{f_{\omega_{m-}}^2}} \end{aligned} \quad (54)$$

with

$$f_{\omega_{m\pm}} = \frac{A + B \pm \sqrt{(A-B)^2 + 4C^*C}}{2(AB - C^*C)}. \quad (55)$$



See the quasiparticle and quasihole dispersions in Fig. 5 (a) and (b). In addition, we also plot the first-order approximations (the minimum values of  $\Delta E_{k,1}$  and  $\Delta E_{k,2}$ , i.e.,  $\Delta E_{k,1m}$  and  $\Delta E_{k,2m}$ ) to the dispersion of the density fluctuations in Fig. 1 (b). Fig. 1 (b) indicates that the band gap disappears as we approach the critical value  $\bar{U}_c/J \approx 8.25$  that is consistent with the result found in Fig. 1 (a). Fig. 5 (a) and (b) also shows that there are Weyl nodes in the Bogoliubov excitation spectra in Mott-insulator phase, and the Mott gap  $E_{k,2m}$  becomes larger as the interaction strength increases similar to that in conventional Bose-Hubbard models.

Next, we apply the BdG theory to study the quasiparticle and quasihole excitations in Mott-insulator phase by choosing a slab with finite width and sharp the boundaries along planes orthogonal to the  $\vec{x}-\vec{y}$  direction. After calculations, we present the results in Fig. 5 (c) and (d). It shows that there are also bosonic surface-arc states at boundaries.

## V. DISCUSSION AND CONCLUSION

We have studied properties of Bogoliubov excitations in systems described by the Bose-Hubbard extension of the WSM. By using Bogoliubov theory, we calculate the energy spectra of excitation modes for the system with weak repulsive interactions, and find they exhibit non-trivial properties with Weyl points. There exist bosonic

surface-arc connected by Weyl points with different chiralities analogs of Fermi arc in WSM of electronic system. As the interaction increases, Weyl points approach gradually with each other along the z-direction.

In the strong coupling regime, the system is in MI phase, where the fluctuation (described as quasiparticle and quasihole excitations) in average number of particles per site goes to zero at the zero temperature. By using a path integral formulation, we calculate the excitation spectra of the MI state. We find that there are two quasiparticle dispersions touching at stable nodes (Weyl points), and there are also bosonic surface-arc at boundaries.

In addition to the type-I WSM considered in this paper, we also expect that there are also novel excitations in the Bose-Hubbard extension of type-II and hybrid WSMs. The bosonic Weyl excitations will deepen our standing of quantum many body physics.

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